Topic 4: Introductory Organic Chemistry and Alkanes

Related topics in Units 2, 4 and 5 will assume knowledge of this material.

4A: Introduction

Students will be assessed on their ability to:

4.1	understand the difference between hazard and risk
	A **hazard** is something that could cause harm to a user A **risk** is the chance of a hazard causing harm
4.2	understand the hazards associated with organic compounds and why it is necessary to carry out risk assessments when dealing with potentially hazardous materials

Risk assessment is the identification of the hazards involved in carrying out a procedure and the control measures needed to reduce the risks from those hazards

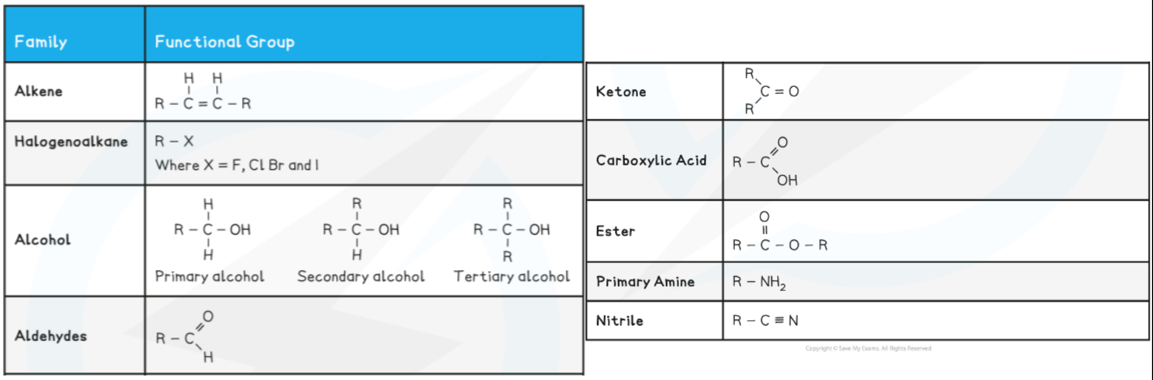
		
Moderate health hazard	**Serious health hazard**	**Toxic (poisonous/ lethal)**
Causes skin irritation	Causes breathing difficulties/ carcinogenic	Could cause death if swallowed or inhaled

		
Flammable	**Oxidising**	**Harmful to the environment**

	
Corrosive	**Explosive**

4.3	be able to suggest ways in which risks can be reduced and reactions carried out safely, for example: i working on a smaller scale ii taking precautions specific to the hazard iii using an alternative method that involves less hazardous substances

4.4	understand the concepts of homologous series and functional group
	A **<u>functional group</u>** is an atom or group of atoms in a molecule/compound that determines its chemical reactions A **<u>homologous series</u>** is a family of compounds with similar chemical properties with the same functional group, same general formula, which differs in molecular formula by CH_2 from the next member, and shows a gradual change in physical properties



Family	Functional Group
Alkene	$R-CH=CH-R$
Halogenoalkane	$R-X$ Where X = F, Cl Br and I
Alcohol	$R-CH_2-OH$ Primary alcohol; $R-CHR-OH$ Secondary alcohol; $R-CR_2-OH$ Tertiary alcohol
Aldehydes	$R-CHO$
Ketone	$R_2C=O$
Carboxylic Acid	$R-COOH$
Ester	$R-CO-O-R$
Primary Amine	$R-NH_2$
Nitrile	$R-C\equiv N$

4.5	be able to apply the rules of International Union of Pure and Applied Chemistry (IUPAC) nomenclature to: i name compounds relevant to this specification ii draw these compounds, as they are encountered in the specification, using structural, displayed and skeletal formulae *Students will be expected to know prefixes for compounds up to C_{10}*
4.6	be able to classify reactions as addition, substitution, oxidation, reduction or polymerisation
4.7	understand that bond breaking can be: i homolytic, to produce free radicals ii heterolytic, to produce ions
4.8	know definitions of the terms ‘free radical’ and ‘electrophile’
	Free radical is a species that contains an unpaired electron **Electrophile** is a species that is attracted to a region of high electron density (they accept a pair of electrons)

A bit of recap from International-GCSE stuff

4B: Alkanes

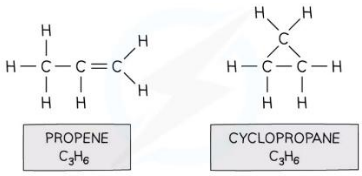
Students will be assessed on their ability to:

4.9	know the general formula of alkanes and cycloalkanes, and understand that they are hydrocarbons (compounds of carbon and hydrogen only) which are saturated (contain single bonds only)
	Hydrocarbon is a compound containing only hydrogen and carbon atoms Alkanes are a group of ***saturated*** hydrocarbons General Formula: $\boxed{C_nH_{2n+2}}$ They are colorless compounds and can be linear, branched or cyclic Cycloalkanes have the general formula C_nH_{2n} This general formula is the same as Alkenes but do note that cycloalkanes are still saturated Alkanes are generally unreactive and their unreactive nature can be explained by: 1. The high bond enthalpies of C-C and C-H bonds Bond enthalpy of C-C is 316 kJ/mol and C-H is 411kJ/mol which means the C-H bond is stronger (This is because hydrogen atom only consists of one shell so the distance between the nuclei is shorter, thus creating greater force of attraction to the nuclei and the pair of electrons between them 2. The very low polarity of the sigma bonds present The electronegativities of carbon and hydrogen are very similar so both C-H bond and C-C bond is non-polar, thus making the overall alkane non-polar
4.10	understand the term 'structural isomerism' and be able to draw the structural isomers of organic molecules, given their molecular formula

Isomerism

Structural isomerism

Same molecular formula but different structural formula



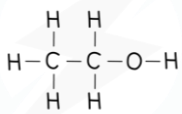
stereoisomerism

Same molecular and structural formula but different arrangements in 3d (will study further in A2)

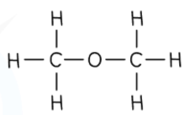
functional group isomerism

Let's consider C_2H_6O

Ethanol



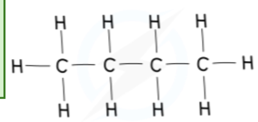
Ether



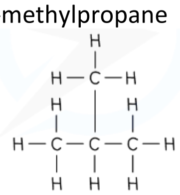
chain isomerism

Let's consider C_4H_{10}

Butane



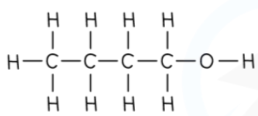
2-methylpropane



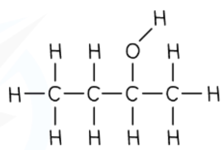
positional isomerism

Let's consider C_4H_9OH

Butan-1-ol



Butan-2-ol



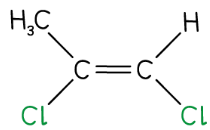
optical isomerism

We will study this further in A2 Unit 4 (stay tuned!)

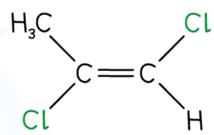
geometric isomerism

Let's consider 1,2-dichloropropene

Z-isomer



E-isomer



4.11	be able to draw and name the structural isomers of alkanes and cycloalkanes with up to six carbon atoms

Methane
1 isomer

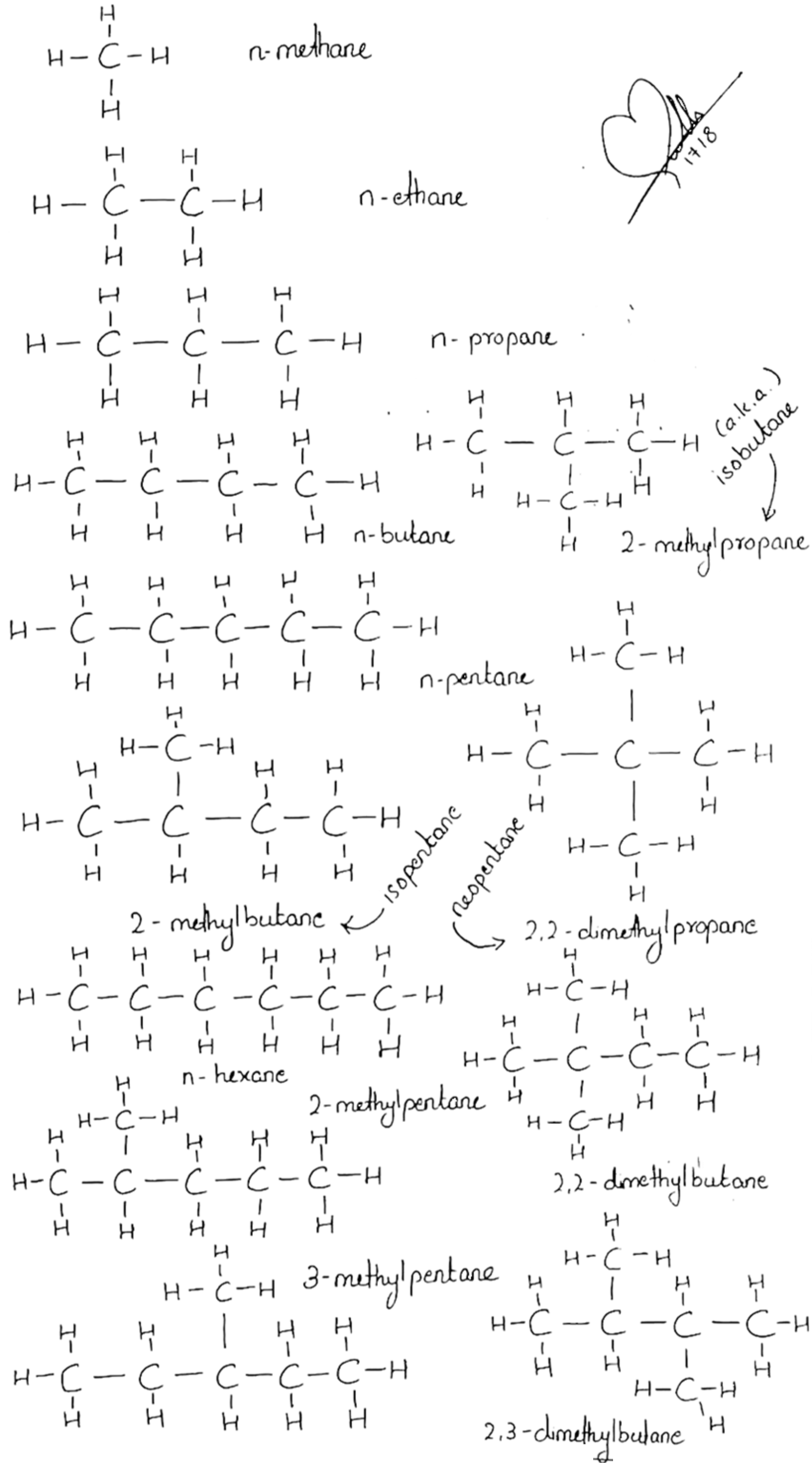
Ethane
1 isomer

Propane
1 isomer

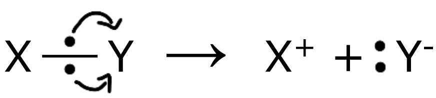
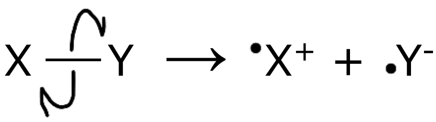
Butane
2 isomers

Pentane
3 isomers

Hexane
5 isomers



4.12	know that alkanes are used as fuels and obtained from the fractional distillation, cracking and reforming of crude oil, and be able to write equations for these reactions
4.13	know that pollutants, including carbon monoxide, oxides of nitrogen and sulfur, carbon particulates and unburned hydrocarbons, are emitted during the combustion of alkane fuels
4.14	understand the problems arising from pollutants from the combustion of alkane fuels, limited to the toxicity of carbon monoxide and why it is toxic, and the acidity of oxides of nitrogen and sulfur

4.15	be able to discuss the reasons for developing alternative fuels in terms of sustainability and reducing emissions, including the emission of CO_2 and its relationship to climate change
4.16	be able to apply the concept of carbon neutrality to different fuels, such as petrol, bioethanol and hydrogen
4.17	understand the reactions of alkanes with: i oxygen in the air (combustion) ii halogens
i	When alkanes are combusted in excess oxygen, ***complete combustion*** takes place Alkane + Oxygen → Carbon dioxide + Water (note that CO_2, a greenhouse gas, is a major contributor to global warming) When alkanes are combusted in a limited supply of oxygen, ***incomplete combustion*** takes place Alkane + Oxygen → Carbon monoxide + Water (or) Alkane + Oxygen → Carbon (soot) + Water (can be seen in car engines)
ii	Alkanes can undergo ***free radical substitution*** with halogens in presence of UV light Mechanism is explained in detail below
4.18	understand the mechanism of the free radical substitution reaction between an alkane and a halogen: i using free radicals, which are species with an unpaired electron, represented by a single dot ii showing the initiation step of the mechanism, with curly half-arrows for free radical formation iii showing the propagation and termination steps of the mechanism iv having limited use in synthesis because of further substitution reactions
i	There are two types of bond fission: Heterolytic Fission & Homolytic Fission  The more electronegative atom takes both the electrons from the bond to form a negative ion (this negative ion is an electron-rich species that can donate a pair of electrons making it a nucleophile) The resulting positive ion is an electron-deficient species that can accept a pair of electrons making it an electrophile  Each atom takes an electron from the bond to form two free radicals (species containing an unpaired electron) But in the case of free radical substitution between an alkane and a halogen, only homolytic fission occurs in the halogen (alkane is too unreactive to be affected by UV) !Note that homolytic bond fission does not only occur in the initiation step but in propagation too where the C-H bond splits homolytically

(c) Heptane, C_7H_{16}, reacts with chlorine in the presence of ultraviolet radiation. 2021 June U1 Q-21

(i) State the type and mechanism of this reaction.

(2)

Free radical substitution

(ii) Give the mechanism for the reaction to produce $C_7H_{15}Cl$, $C_{14}H_{30}$ and HCl as the **only** products.

Include the name of each of the steps in your mechanism.

Curly half-arrows are **not** required.

(7)

Free radicals are very reactive and will attack the unreactive alkanes

Initiation Step: $Cl-Cl \xrightarrow{UV} Cl^{\bullet} + Cl^{\bullet}$

An alkyl free radical is produced

Propagation Step:

A C-H bond breaks homolytically

$C_7H_{16} + Cl^{\bullet} \longrightarrow C_7H_{15}^{\bullet} + HCl$

$C_7H_{15}^{\bullet} + Cl_2 \longrightarrow C_7H_{15}Cl + Cl^{\bullet}$

Termination Step: $Cl^{\bullet} + Cl^{\bullet} \longrightarrow Cl_2$

$C_7H_{15}^{\bullet} + Cl^{\bullet} \longrightarrow C_7H_{15}Cl$

$C_7H_{15}^{\bullet} + C_7H_{15}^{\bullet} \longrightarrow C_{14}H_{30}$

$C_7H_{15}Cl + Cl_2 \longrightarrow C_7H_{14}Cl_2 + HCl$

$C_7H_{14}Cl_2 + Cl_2 \longrightarrow C_7H_{13}Cl_3 + HCl$

$C_7H_{13}Cl_3 + Cl_2 \longrightarrow C_7H_{12}Cl_4 + HCl$

Repeat until all H atoms have been substituted .....

$C_7HCl_{11} + Cl_2 \longrightarrow C_7Cl_{16} + HCl$

In *excess halogen (chlorine in this case)* in the presence of UV light, *further substitution* can take place which will produce more products which means it has limited use in synthesis of organic compounds

Further suggested practical

Cracking alkanes by thermal decomposition, including liquid paraffin using aluminium oxide as a catalyst

Topic 5: Alkenes

Related topics in Units 2, 4 and 5 will assume knowledge of this material.

Students will be assessed on their ability to:

5.1 know the general formula of alkenes and understand that alkenes and cycloalkenes are hydrocarbons which are unsaturated (have a carbon-carbon double bond which consists of a σ bond and a π bond)

All alkenes contain a C=C double bond so they are all unsaturated compounds

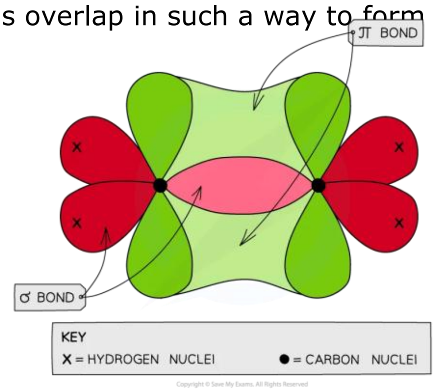
General Formula: $\boxed{C_nH_{2n}}$

The fact that they contain a C=C bond means they are more reactive than alkanes

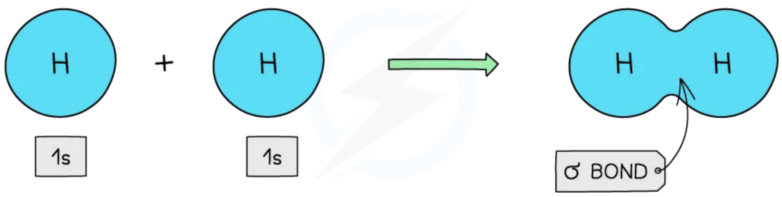
Cycloalkenes have the general formula C_nH_{2n-2}

When forming a covalent bond, the orbitals overlap in such a way to form two types of bonds: sigma and pi bonds

π bonds (a.k.a C=C double bonds) are exposed and have high electron density hence they are more vulnerable to attack by electrophiles (electron-loving species)

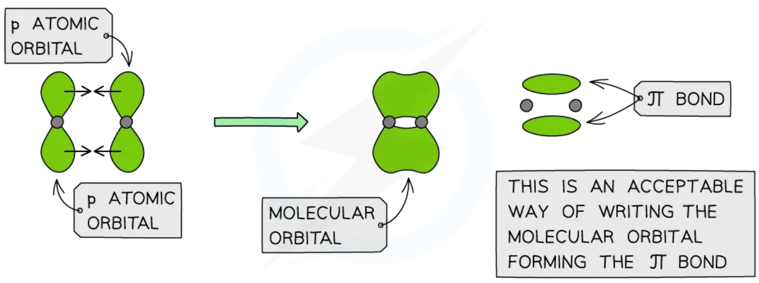


<u>Formation of a (σ) sigma bond</u>



- Sigma bonds are formed from the end to end overlap of atomic orbitals (this is true for both s and p orbitals)
- Rotation can occur around a sigma bond

<u>Formation of a (π) pi bond</u>



- *Pi bonds are formed from the sideways overlap of adjacent p orbitals*
- A single pi bond has two-electron clouds, one above and one under the plane of the sigma bond (each electron cloud representing one bond containing two electrons)
- This arrangement maximises the overlap of the p-orbitals

5.2 be able to explain geometric isomerism in terms of restricted rotation around a C=C double bond and the nature of the substituents on the carbon atoms

In saturated compounds, the atoms/functional groups attached to the single, σ-bonded carbons are not fixed in their position due to the free rotation about the C-C σ-bond

In unsaturated compounds, the groups attached to the C=C carbons can only be in one of two positions, and they remain fixed in that position